

Influence of the Pauli exclusion principle on scattering properties of cobosons

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We examine the influence of the Pauli exclusion principle on the scattering properties of composite bosons (cobosons) made of two fermions, such as the exciton quasiparticle. The scattering process incorporates boson-phonon interactions that arise due to lattice vibrations. Composite boson scattering rates increase with the entanglement between the two fermionic constituents, which comes with a larger number of available single-fermion states. An important role is played by probabilities associated with accommodating an incoming boson among the remaining unoccupied Schmidt modes in the initial composite system. While due attention is given to bi-fermion bosons, the methodology is applicable to any composite boson made up of smaller boson fragments. Due to super-bunching in a system of multiple boson condensates such as bi-bosons, there is enhanced scattering associated with bosons occupying macroscopically occupied Schmidt modes, in contrast to the system of bi-fermion pairs.

I. INTRODUCTION

Composite bosons¹⁻⁷ that fall within the spectrum bounded by ideal bosons and fermions have been the subject of many recent works⁸⁻¹⁷. While several bosons may occupy the same state, multiple occupation is inhibited in the case of two fermions, due to the Pauli exclusion principle. The difference between bosons and fermions is reflected in all basic and experimental studies due to the symmetrization postulate, and interferences that arise through the superposition principle. For composite boson made of an even number of fermions, also known as “cobosons”^{3,4}, the Pauli principle does not influence the dynamics of the two highly entangled fermions. In this case, the constituent fermions seldom compete for single-particle states. The Pauli principle, although still omnipresent, therefore does not influence composite bosons with low occupation probabilities. A range of phase-space filling effects and commutation relations arise due to the emergence and pronounced governance of the Pauli principle beyond a critical level of occupation probabilities of the constituents of the coboson species.

Recent studies on composite bosons made of two distinguishable entangled constituents such as the two-fermion boson system, have shown the subtle links between entanglement and indistinguishability, through the diminishing effects of the Pauli exclusion principle with increase in entanglement^{4,6-8,10,11,18}. The term “entanglement” refers to the situation in which individual non-interacting constituents of a quantum system are influenced by one another, with a collective wavefunction describing the quantum properties of the system. An algebraic description of composite bosons from the perspective of quantum information^{4,6,7} provides insight to the microscopic quantum description of many body systems. The purity P of the single-particle density matrix is a quantitative indicator for entanglement of a system of constituent fermions^{4,6,7}. Deviations from unity of the ratio, $\alpha_{N+1} = \sqrt{\chi_{N+1}/\chi_N}$, to be defined below, where χ_N is the normalization term associated with N cobosons, provides a measure of “compositeness” of systems of boson and fermion constituents^{4,6,7}. Composite bosons with minimal deviations can be approximated as ideal bosons. The upper and lower bounds to χ_N in terms of the purity P of the single-fermion reduced state, show convergence at small purities^{4,6,7,10,11,15}. At higher purities, the bounds become inefficient^{15,18-20} as factors other than P may control the behavior of the composite bosons. Tighter bounds for the normalisation factor χ_N and for the normalisation ratio χ_{N+1}/χ_N for two-fermion cobosons were recently obtained in terms of the purity P and the largest eigenvalue λ_1 of the single-fermion density matrix²⁰. Due to incorporation of more information through P and λ_1 , the improved results²⁰ enabled convenient evaluation of the normalisation factor at large composite numbers N .

In our earlier works²¹⁻²³, the composite nature of excitons was neglected, partly due to the simplicity and effectiveness of the ideal boson description of the exciton system at low densities^{24,25}. When the mean inter-excitonic distance greatly exceeds the exciton Bohr radius, the correlated electron-hole quasi-particle can be considered structureless. The assumption of the spin independent exciton model breaks down when the dynamics of interacting excitons is influenced by the Pauli exclusion principle. Further neglect of Pauli exclusion as the inter-exciton separation is decreased, will result in increased non-Hermitian features which may distort computed exciton lifetimes. Combescot and coworkers have proposed a “commutator formalism”³ to incorporate the inter-excitonic Pauli exclusion scatterings which are critical to explaining optical features not associated with coulombic interactions between fermions.

The case of the high-density electron-hole system with excitonic instability has also been studied using techniques based on the generalized random-phase approximation²⁶, and the vertex-equation extension²⁷ of the Bardeen, Cooper, and Schrieffer (BCS) theory^{28,29}. In a recent work, Koinov³⁰ employed the BCS and Bethe-Salpeter equations to highlight the appearance of a secondary peak in the optical spectrum that can be linked to an excitonic phase of high density. Imamoglu³¹ examined the limitations imposed by Pauli exclusion of fermions in exciton-phonon interactions, and obtained results showing a dependence

of scattering times on the density of the composite fermionic species. In this work, we examine the influence of the Pauli exclusion principle during scattering of the bi-fermion excitons by phonons which arise from lattice vibrations. We focus on the entanglement attributes of the scattered composite boson system, thereby extending the earlier work of Imamoglu³¹, to include quantum information theoretic factors such as purity, P , and the normalization ratio of composite-boson states. This approach will provide a realistic assessment of the Pauli exclusion effects on the lifetimes of the scattered excitons at high densities of correlated electron-hole pair systems.

The results of this work will also be of interest to composite boson systems that are made of two distinguishable bound bosonic constituents, otherwise known as bi-boson composites¹⁹. Based on the interplay of interactions between boson constituents and the global composite, bi-bosons may operate in the super-bosonic phase in which the boson constituents display enhanced bunching¹⁹. A bunching process is associated with the tendency for particles to be distributed in preferred collective modes instead of a random Poissonian type distribution. In super-bunching, a specific mode for boson occupation is preferred at the expense of other modes. As the number of composite boson is increased, a single mode occupied by a boson attracts further occupation which results in macroscopic occupation of bosons in the preferred mode¹⁹. The super-bunching behavior therefore reduces the occupation of bosons present in other modes.

There results obtained for bi-bosons may be applied to complex aggregate systems containing several electron-hole pairs. In a recent work³², electron-hole aggregates were seen to give rise to a new form of stable quasiparticle states known as quantum droplets. A correlated electron-pair aggregate of large size (ten times the size of a single exciton) in GaAs³² was observed using experimental techniques. The minimum requirement of four electron-hole pairs for stability is novel as the electrons and holes exist in unpaired configurations, yet the quantum droplet appear as a collective boson entity.

This paper is organized as follows. In Section II we provide a brief review of the physics of cobosons, and examine the characteristics of the lower and upper limits to the normalisation ratio in composite boson systems. In Section II B, we discuss the subtle difference between the electron-hole pair numbers and the boson number, and provide a physical interpretation of the number-operator for composite bosons. We also examine the conditions under which an orthogonal fermionic fragment state is formed when a coboson dissociates into constituents in orthogonal subspaces. In Section III, we derive expressions related to the fluctuation to the mean number of correlated coboson constituents. In Section IV, we examine the BCS variational ansatz in the context of excitonic systems, and establish the links between the BCS state parameters, purity P and the normalization ratio α_{N+1} . Using the results in Section IV A, we obtain the scattering rate of composite exciton condensates due to lattice vibrations in Section IV B, with our main result showing the dependence of this rate on the normalization ratio. In Section V, the composite boson made of two bound bosonic constituents or bi-boson systems is examined qualitatively in the context of the findings in Section IV. We present our conclusion in Section VI

II. COBOSONS STATES : PRELIMINARIES

The creation operator of a coboson made of distinguishable fermions can be written in the Schmidt decomposition as^{4,6,7}

$$\hat{c}^\dagger = \sum_{j=1}^S \sqrt{\lambda_j} \hat{a}_j^\dagger \hat{b}_j^\dagger =: \sum_{j=1}^S \sqrt{\lambda_j} \hat{d}_j^\dagger, \quad (1)$$

where λ_j are the Schmidt coefficients, \hat{a}_j^\dagger and \hat{b}_j^\dagger are fermion creation operators associated with each Schmidt mode, and S denotes the total number of Schmidt coefficients³³. The operator \hat{d}_j^\dagger creates a bi-fermion product state in the mode j , hence the operator \hat{c}^\dagger appears as a weighted superposition of all bi-fermion operators that are distributed among the Schmidt modes for the two constituents operators, \hat{a}_j^\dagger and \hat{b}_j^\dagger . The distribution of $\lambda_j = \bar{\Lambda} = (\lambda_1, \dots, \lambda_S)$ ($\lambda_1 \geq \lambda_2 \geq \dots \geq 0$) fulfills $\sum_{j=1}^S \lambda_j = 1$. The purity $P = \sum_{j=1}^S \lambda_j^2$ is related to the Schmidt number K ³⁴ via $K = 1/P$, where the latter quantifies the correlations between the fermions. In the case of the exciton, a large K implies a highly correlated electron-hole pair linked to high binding energies. A less tightly bound exciton is linked to a more distinguishable (and less entangled) electron and hole system.

The operators, \hat{c} and \hat{c}^\dagger obey the approximately bosonic commutation relations

$$\begin{aligned} [\hat{c}, \hat{c}] &= [\hat{c}^\dagger, \hat{c}^\dagger] = 0, \\ [\hat{c}, \hat{c}^\dagger] &= 1 + t \sum_{k=1}^S \lambda_k (\hat{a}_k^\dagger \hat{a}_k + \hat{b}_k^\dagger \hat{b}_k), \end{aligned} \quad (2)$$

with $t = 1$ ($t = -1$) for bi-bosons (bi-fermions). This results in differences between cobosons, depending on their constituents (bosons or fermions).

The state of N composite bosons can be expressed as a superposition of N bi-fermions or N bi-bosons as follows^{6,15,19}

$$|N\rangle = \frac{1}{\sqrt{N!\chi_N^J}} |\psi_N\rangle = \frac{1}{\sqrt{N!\chi_N^J}} (\hat{c}^\dagger)^N |0\rangle \quad (3)$$

where the normalization factor is given by $\chi_N^J = \chi_N^B$ (χ_N^F) in the case of bi-bosons (bi-fermions). The states $|\psi_N\rangle = (\hat{c}^\dagger)^N |0\rangle$ are not normalized as $\langle\psi_N|\psi_N\rangle = N!\chi_N$. The deviations from ideal boson characteristics are incorporated in the normalization term χ_N obtained using $\langle N|N\rangle=1$ as⁴⁻⁷

$$\chi_N^B = N! \sum_{1 \leq j_1 \leq j_2 \leq \dots \leq j_N}^S \prod_{k=1}^N \lambda_{j_k}, \quad (4)$$

$$\chi_N^F = N! \sum_{1 < j_1 < j_2 < \dots < j_N}^S \prod_{k=1}^N \lambda_{j_k}, \quad (5)$$

where $\chi_N^B = \chi_N^F = 1$ for ideal bosons at all N , and $\chi_N^F = 0$ when the number of bi-fermions, N , exceeds the number of available fermionic single-particle states, S . For bi-fermion bosons, χ_N^F can be interpreted combinatorially as the probability associated with N entities yielding different outcomes, when a property j ($1 \leq j \leq S$) is assigned to each entity. There are however differences between the two species as multiple occupation of modes are forbidden in bi-fermions unlike in the case of bi-bosons which are diverse in terms of the occupation profile of the Schmidt modes. In general, it is difficult to compute exactly the normalization factor for both bi-fermions and bi-bosons.

A. Upper and a lower bound to the normalization ratio

A simple inequality involving the upper and a lower bound to the normalization ratio, which yields a measure of departure from ideal boson properties, was obtained as⁷

$$1 - P \cdot N \leq \frac{\chi_{N+1}}{\chi_N} \leq 1 - P, \quad (6)$$

where the lower bound decreases monotonically with N , and vanishes at $P = \frac{1}{N}$. The corresponding uniform state $\vec{\Lambda}^U$ arises from a finite number ($\frac{1}{P}$) of Schmidt modes, with $\chi_{\frac{1}{P}+1} = 0$. The normalization ratio is minimized by a uniform distribution $\vec{\Lambda}^U$. The state associated with the N -independent upper bound in Eq. 6 remains unsaturated as the real, saturable upper bound is smaller than $1 - P$. The bound $1 - P$ provides saturable form for the corresponding state at $N = 1$. By determining the Schmidt coefficients of those states that extremize the normalization ratio, a quantitative indicator for bosonic behavior can be determined in terms of the purity P and the number of composites in the same state N ^{7,15},

$$1 - P \cdot N \leq \frac{\chi_{N+1}}{\chi_N} \leq 1 - \frac{PN}{1 + (N-1)\sqrt{P}}. \quad (7)$$

These bounds will be useful in estimating physical quantities such as scattering rates, and other processes in which the number of cobosons N and single-fermion states S remain large.

B. Number-operator for composite bosons

The physical interpretation of the mean number operator \hat{N} defined as

$$\hat{N} = \hat{c}^\dagger \hat{c} =: \sum_{j,k=1}^S \sqrt{\lambda_j \lambda_k} \hat{d}_j^\dagger \hat{d}_k, \quad (8)$$

is only unambiguous when the constituents are highly entangled. However, with increasing deviations from the ideal commutation relation, this expectation value operator yields a boson number that is less than the total number of bi-fermions provided by the number-conserved operator

$$\hat{n}_{tot} = \sum_{j=1}^S \hat{n}_j. \quad (9)$$

While \hat{n}_j measures the number of bi-fermions or bi-bosons in a single mode, j , it is not influenced by the bosonic quality or entanglement attributes of the composite bosons. The operator, \hat{n}_j is number-conserving as the number of bi-fermions is conserved under all dynamical processes, which includes those that unbind the constituents into freely existing form. The apparent loss in the boson number which appears in the mean number operator \hat{N} , can be attributed to transitions of non-ideal fermionic fragments to orthogonal subspaces which accommodate non-ideal states orthogonal to all other states $|M\rangle$ with $M = 0, \dots, N$. The expectation value of the number operator \hat{N} yields the number of bi-fermions that exist as correlated entities, which differs from the interpretation of \hat{n}_{tot} in Eq. 9 which obeys an invariance in the boson number. In this regard, the term “number” holds different meanings for the two operators, \hat{N} and \hat{n}_{tot} , with the former operator associated with the total number of composite bosons which are entangled or remain correlated. On the other hand, \hat{n}_{tot} includes all constituents of the coboson, independent of their state of correlation or existence as free fermions. Here we employ \hat{N} as a coboson number operator that quantifies only the correlated electron-hole pairs, and which is amenable to change with environmental conditions. We also utilize this operator within the BCS wave function ansatz associated with a grand canonical ensemble to analyze the scattering of excitons examined in this study.

In material systems such as semiconductors, the coboson operator \hat{N} effectively differentiates strongly bound bosonic excitons from free electron-hole pairs. With increase in fermion densities, the actual number of bi-fermion pairs that can be treated as ideal bosons³⁵ decreases, this is reflected in a decreased expectation of \hat{N} associated with lower normalization ratios of the quantum state of N composites. The difference between \hat{N} and \hat{n}_{tot} can be taken as a measure of the non-ideal nature of cobosons. For bi-fermions, we can set $\hat{n}_j = \hat{d}^\dagger \hat{d}$ as each mode can only be occupied by at most a single bi-fermion. The scenario is different in the case of bi-bosons as each mode j can be occupied by several particles. The expectation value of $\hat{d}^\dagger \hat{d}$ yields n_j^2 instead of n_j . As a consequence, the expectation value of \hat{N} for bi-boson composites can be larger than the actual number of bi-bosons, for which a physical interpretation is desirable. These differences highlight the challenges in treating bi-bosons in the same footing as bi-fermion cobosons. We therefore pay greater attention to the scattering of bi-fermion condensates in this work, and consider the bi-bosons on qualitative terms in Section V.

C. Formation of a fermionic fragment

The process in which a particle is removed from a coboson condensate occurs in a total Hilbert space that is decomposed into two orthogonal subspaces. One subspace holds the boson condensate while the other is occupied by the orthogonal fragment species. The Fock-space with N bi-fermions is made up of an N -coboson-state and a fermionic non-ideal state that is orthogonal to all coboson states. The action of the creation operator, \hat{c}^\dagger (Eq. 1) on a N -composite bosons state can be derived as

$$\hat{c}^\dagger |N\rangle = \frac{\hat{c}^\dagger}{\sqrt{N! \chi_N}} |\psi_N\rangle = \frac{1}{\sqrt{N! \chi_N}} |\psi_{N+1}\rangle = \alpha_{N+1} \sqrt{N+1} |N+1\rangle \quad (10)$$

where $\alpha_N = \sqrt{\chi_N / \chi_{N-1}}$. The $|N\rangle$ state constitutes a subset of the entire Hilbert space associated with the constituent particles, thus the action of \hat{c} on $|N\rangle$ appears as

$$\hat{c} |N\rangle = A_N |N-1\rangle + |\varepsilon_N\rangle \quad (11)$$

where $|\varepsilon_N\rangle$ denotes the fragment state that is orthogonal to $|N-1\rangle$. The constant A_N is obtained using 10 as

$$A_N = \langle N-1 | \hat{c} | N \rangle = \alpha_N \sqrt{N}. \quad (12)$$

The state $|\varepsilon_N\rangle$ in Eq. 11 is orthogonal not only to the state $|N-1\rangle$, but also to any state $|M\rangle$ with $M = 0, \dots, N^6$, hence $\langle M | \varepsilon_N \rangle = 0$ for $M = 0, \dots, N$. The correction factor, $\langle \varepsilon_N | \varepsilon_N \rangle$ has been obtained as^{4,6}

$$\langle \varepsilon_N | \varepsilon_N \rangle = 1 - \frac{\chi_{N+1}}{\chi_N} - N \left(\frac{\chi_N}{\chi_{N-1}} - \frac{\chi_{N+1}}{\chi_N} \right). \quad (13)$$

For ideal bosons, $\langle \varepsilon_N | \varepsilon_N \rangle \rightarrow 0$, and in the case of bi-fermion cobosons such as excitons, the increased densities of electron-holes pairs will result in a higher correction factor, as the ratio, α_N is strictly non-increasing with N^7 .

III. FLUCTUATION TO THE MEAN NUMBER, $\langle \hat{N} \rangle$ OF BI-FERMIONS

In the context of the scattering process to be examined in this work, the fluctuations in the mean number of correlated coboson constituents, $\langle \hat{N} \rangle$ present as an important factor which quantifies changes that may occur during dynamical interactions with

external entities such as phonons. While the fluctuations measures changes in the correlated coboson constituents, it is possible that the total number of fermion pairs (as measured by \hat{n}_{tot} in Eq. 9) may be altered due to recombination effects that result in phonon emission. In this work, we assume that such recombination effects are minimal, and focus on the influence of the normalization ratio on $\langle \hat{N} \rangle$ and fluctuations associated with the number of correlated bi-fermion pair systems.

In an earlier work examining the commutation relations involving cobosons^{1,2}, a relation was obtained as

$$\hat{c}^\dagger \hat{c} |\psi_N\rangle = |\psi_N\rangle + \frac{N-1}{N+1} \hat{c} |\psi_{N+1}\rangle \quad (14)$$

Eq. 14 is useful both in the calculation of the effective mean number, $\langle \hat{N} \rangle$ of bi-fermions and in seeking extensions of the trilinear commutation relations³⁶⁻³⁸ to coboson systems. Using Eq. 14 we obtain

$$\langle \hat{N} \rangle = \langle N | \hat{c}^\dagger \hat{c} | N \rangle = \frac{\langle \psi_N | \hat{c}^\dagger \hat{c} | \psi_N \rangle}{\langle \psi_N | \psi_N \rangle} = 1 + (N-1) \frac{\chi_{N+1}}{\chi_N} \quad (15)$$

$$\langle \hat{N}^2 \rangle = \frac{\langle \psi_N | \hat{c}^\dagger \hat{c} \hat{c}^\dagger \hat{c} | \psi_N \rangle}{\langle \psi_N | \psi_N \rangle} = 1 + \left(\frac{(N-1)^2}{N+1} + 2N-2 \right) \frac{\chi_{N+1}}{\chi_N} + \frac{N(N-1)^2}{N+1} \frac{\chi_{N+2}}{\chi_N} \quad (16)$$

where $\langle \hat{A} \rangle = \langle N | \hat{A} | N \rangle = \langle \psi_N | \hat{A} | \psi_N \rangle / \langle \psi_N | \psi_N \rangle$ is the mean value of the operator \hat{A} and $\hat{N} = \hat{c}^\dagger \hat{c}$ is considered the cobosons number operator. We reiterate, as discussed in Section II B, that \hat{N} quantifies the number of excitons (or correlated bi-fermions) and is not inclusive of the free electron-hole pairs which result from the scattering process to be considered shortly.

For moderate values of the purities, $P = \frac{\gamma}{N}$ where $\gamma < 1$, we obtain using Eqs. 15 and 16, the fluctuation in the mean number, $\langle \hat{N} \rangle$ as follows

$$\left[\frac{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2}{\langle \hat{N} \rangle^2} \right]_{\frac{\chi_{N+1}}{\chi_N} = 1-P} = \frac{\gamma(N-1)^2(N-\gamma)}{(N+1)(\gamma + N^2 - \gamma N)^2} \quad (17)$$

$$\left[\frac{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2}{\langle \hat{N} \rangle^2} \right]_{\frac{\chi_{N+1}}{\chi_N} = 1-NP} = \frac{\gamma(N-1)^2(\gamma + (\gamma-1)N)}{(N+1)((\gamma-1)N^2)^2 - \gamma} \quad (18)$$

with the fluctuations vanishing in the limit $P \rightarrow 0$, and increasing gradually with P . The expression for $\langle \hat{N} \rangle$ at the tighter upper bound (see Eq. 7) is lengthy, and therefore we do not include its form here. While the bounds on χ_N also bound \hat{N} , this property does not extend to the case of the fluctuations in the mean number, $\langle \hat{N} \rangle$. The (normalised) second order correlator $g_N^{(2)}$ characterizes the probability of detecting of particles at times t and $t + \tau$ ^{39,40}

$$g_N^{(2)}(\tau) = \frac{\langle \hat{c}^\dagger(t) \hat{c}^\dagger(t+\tau) \hat{c}(t+\tau) \hat{c}(t) \rangle}{\langle \hat{N}(t) \rangle \langle \hat{N}(t+\tau) \rangle} \quad (19)$$

Eq. 19 can be interpreted as a measure of correlations between N cobosons, with exclusion of all free fermion constituents, and takes into account the time-dependence of creation and annihilation operators. $g_N^{(2)}(\tau)$ is not directly interpretable in terms of the normalization ratio, $\frac{\chi_{N+1}}{\chi_N}$ and purity, P due to the time independence of the latter quantities. It is therefore appropriate to consider the second order correlation function at zero time delay, $g_N^{(2)}(0)$ which provides information on the underlying statistical features, such as the Poissonian case ($g_2(0) = 1$) in coherent systems involving a large number of Fock states. $g_N^{(2)}(0)$ is a useful indicator of the bosonic quality and may be used to monitor rate changes during scattering processes involving cobosons. $g_N^{(2)}(0)$ is rewritten using Eq. 19 as

$$g_N^{(2)}(0) = \frac{\langle \hat{c}^\dagger \hat{c}^\dagger \hat{c} \hat{c} \rangle}{\langle \hat{c}^\dagger \hat{c} \rangle^2} \quad (20)$$

The full derivation of $g_N^{(2)}(0)$ and analysis of its upper and lower bounds will be considered elsewhere, however we will refer to its utility in connection with the BCS variational ansatz in Section IV A.

IV. SCATTERING OF COMPOSITE EXCITON CONDENSATES DUE TO LATTICE VIBRATIONS

A. The BCS variational ansatz

The typical exciton creation operator with the center-of-mass momentum K and an internal motion associated with the $1s$ state can be written as^{21–23,25}

$$C_K^\dagger = \sum_{k_e, k_h} \delta_{K, k_e + k_h} \phi_{1s}(\alpha_e k_h - \alpha_h k_e) a_{k_e}^\dagger h_{k_h}^\dagger \quad (21)$$

where the spin parameters have been dropped for simplicity and $\alpha_e(\alpha_h) = \frac{m_e}{M}(\frac{m_h}{M})$, where m_e (m_h) is the electron (hole) mass and M is the total mass of the carriers. The electron (hole) wavevectors k_e (k_h) in Eq. 21 spans the Brillouin zone in the momentum space. a_k^\dagger and h_k^\dagger denote the respective electron and hole creation operators, which are linked as

$$h_k^\dagger = a_{-k} \quad (22)$$

In Eq. 21, $\phi_{1s}(\alpha_e k_h - \alpha_h k_e)$ denotes the $1s$ wavefunction of a hydrogen type system, which depends on the relative electron-hole separation in real space. The excitonic wavefunction can be written as

$$|\Phi_{ex}\rangle = C_K^\dagger |0\rangle \quad (23)$$

where the vacuum state $|0\rangle$ denotes a completely filled valence band, and an empty conduction band.

A mean-field description of the exciton condensate, analogous to the Bardeen-Cooper-Schrieffer (BCS) form⁴¹ is suitable to model a system of interacting fermions^{42–44}. The wavefunction of the composite condensate of bi-fermion pairs with zero center-of-mass momentum appears in a normalized form^{42–44}

$$|\Phi_{BCS}\rangle = \prod_k \left[u(k) + v(k) a_k^\dagger h_{-k}^\dagger \right] |0\rangle, \quad (24)$$

where the coefficients, $u(k), v(k)$ satisfy the normalization condition, $u^2(k) + v^2(k) = 1$. A small ratio $\frac{v(k)}{u(k)} = \phi_k \ll 1$ applies at the low-density range of the bi-fermion system at which $u(k) \approx u(0) = 1$ for all k . Eq. 24 represents a state in which the constituents of the bi-fermion pair ($a_k^\dagger, h_{-k}^\dagger$) are either both present or absent, hence the species remain correlated for the lifetime of the bi-fermion complex. The ground state becomes separable only if either $u(k) = 1$ or $v(k) = 1$ for all k , however, the values of $|v(k)|^2$ for which the correlated electron-hole pair system retains its excitonic features is not apparent in Eq. 24. This state changes from a system of excitonic boson gas to that of a two-component plasma present at high fermion densities. Such a change is dependent on system parameters such as the size of confinement, exciton Bohr radius, and density of fermion pairs. The number of coboson particles is therefore not fixed for the state in Eq. 24. In the case of the dilute bi-fermion condensates, $\sum_k |v(k)|^2 = \sum_k \frac{\phi_k^2}{(1+\phi_k^2)} \approx N(\frac{a_B}{L})^3$ where a_B is the exciton bohr radius, L is the confinement length and $\phi_{1s}(k)$ is the wavefunction in a three-dimensional momentum space given by $\phi_{1s}(k) = \sqrt{64\pi a_B^2}/[1 + (ka_B)^2]^2$. For the reduced units, $a_B=L=1$, $\sum_k |v(k)|^2 = N_t$, the total number of bi-fermions pairs in the ground state.

The overlap term, $\mathcal{O} = |u^*(k) v(k)|$ deserves special mention as it is determined by the coherence between the bi-fermion pairs. This term assumes a significance role in electronic properties of the condensate, and it will be shown to influence the scattering properties due to lattice vibrations (Section IV B), and the dynamics of growth of the bi-fermion condensate. The negativity $\mathcal{N}(k) = u(k) v(k)$ was proposed⁴⁵ as an entanglement measure of the interacting charge carriers using

$$E_N(BCS) = \sum_k \log[\mathcal{N}(k)] = \sum_k \log[u(k) v(k)] \quad (25)$$

The negativity⁴⁶ is equivalent to another well known entanglement measure known as the concurrence, \mathcal{C} . The concurrence measure \mathcal{C} for the qubit state ($u|00\rangle + v|11\rangle$) appear as $2uv$. The two entanglement measures (\mathcal{N}, \mathcal{C}) may be treated as thermodynamical attributes of the BCS wave function ansatz associated with a grand canonical ensemble of a fixed chemical potential. Both measures can be compared to the ratio, $\frac{\chi_{N+1}}{\chi_N}$ which quantifies the entangled state of N coboson state. The maximally entangled state is described by $\mathcal{N}=1$ correlates with the ideal boson state, $\frac{\chi_{N+1}}{\chi_N}=1$.

In a dilute system of bi-fermion pairs, the relation $\sum_k |u^*(k) v(k)|^2 \approx \sum_k |v(k)|^2$ can be employed to estimate the overlap term, $\mathcal{O}^2 = \sum_k |u^*(k) v(k)|^2$. Using the effective mean number, $\langle \hat{N} \rangle$ of bi-fermions in Eq. 15 we obtain

$$\sum_k |u^*(k) v(k)|^2 = \langle N | \hat{c}^\dagger \hat{c} | N \rangle = N \alpha^2_{N+1} = N \frac{\chi_{N+1}}{\chi_N} \quad (26)$$

which is applicable in systems of low purity, P . Eq. 26 can be understood by noting that the coherence between the bi-fermions is diminished as a result of the addition of the $(N + 1)$ st coboson due to the Pauli principle occurring with the likelihood of $1 - \frac{\chi_{N+1}}{\chi_N}$. The system of bi-fermions will have enhanced \mathcal{O}^2 for entangled fermions where there is no competition for single-fermion states due to the Pauli principle. The overlap term \mathcal{O}^2 is expectedly maximized in a system with purity, $P = 0$ (see Eq. 6). It is to be noted that Eq. 26 is based on the assumption that the system of electron-hole pairs is dilute and highly entangled (with low P values). This allows the results from the normalization factor of N -identical composite boson state to be linked to parameters of the BCS wave function ansatz as shown in Eq. 26.

The overlap term \mathcal{O}^2 can also be estimated using the second order correlation function at zero time delay, $g_N^{(2)}(0)$ given in Eq. 20. An analytical form for \mathcal{O}^2 can thus be obtained by noting a simple form of the bosonic quality term⁴⁰ obtained using $g_N^{(2)}(0) = \frac{\gamma_{N-1}^2 \gamma_N^2}{N^2}$. In the case of excitons with bohr radius a_B placed in quantum dots of size L , with small values of $\frac{a_B}{L}$ and $N \ll \frac{L}{a_B}$, $\gamma_N = \sqrt{N} \sqrt{1 - 2(N-1)(\frac{a_B}{L})^2}$. Using $g_N^{(2)}(0)$ to estimate \mathcal{O}^2 , we obtain the approximate relation

$$\sum_k |u^*(k) v(k)|^2 = \alpha^2_{N+1} \approx N \left(1 - \frac{2 N a_B^2}{L^2} \right), \quad (27)$$

which is applicable to a system of N bosons in quantum dots with small $\frac{a_B}{L}$. The role of a similar term in an earlier work on the scattering of composite bosons has been discussed in Ref.³¹. Using Eq. 27, we note that at larger $\frac{a_B}{L}$ values, increased confinement effects yields diminished number of correlated electron-hole pairs due to the Pauli exclusion principle. An increase in the fermionic fragment size coupled with a Mott-like transition occurs at higher densities, and results in the formation of an electron-hole plasma state. Hence increased deviations from the ideal boson characteristics due to a decrease in quantum dot size gives rise to a reduced coherence features due to lower values of \mathcal{O}^2 .

B. Rate of Scattering of composite exciton condensates

We consider a process in which an initial state of an exciton and a composite condensate of N bi-fermion pairs gets scattered to a final state of $N + 1$ bi-fermions pairs, with emission of a phonon³¹. The schematics of the channel is shown in Fig 1. The momentum remains conserved when the exciton plus condensate ($C(0, N)$) system is scattered to a final state of $(N + 1)$ bi-fermion pairs, ($C(0, N+1)$), with creation of phonon with wavevector, $K - K'$ as follows

$$\text{Ex}(K) + C(0, N) \rightarrow C(K', N + 1) + \text{phonon}(K - K') \quad (28)$$

The energy of the emitted phonon (with momentum $K - K'$) is derived from the energy released when the exciton coalesces with the condensate of bi-fermions. The final state of bi-fermion condensate acquires a net momentum of K' . The composite exciton Hamiltonian in contact with a phonon reservoir reads²¹

$$\mathcal{H}_T = \mathcal{H}_{ex} + \mathcal{H}_p + \mathcal{H}_{ep}, \quad (29)$$

$$\mathcal{H}_p = \sum_q \hbar \omega(q) b_q^\dagger b_q, \quad (30)$$

$$\mathcal{H}_{ep} = N^{-1/2} \sum_{k,q} (\chi_e(q) a_{k+q}^\dagger a_k + \chi_h(q) h_{k+q}^\dagger h_k) (b_{-q}^\dagger + b_q),$$

where the exciton Hamiltonian \mathcal{H}_{ex} is given by $\sum_k E_0(k) C_k^\dagger C_k$ and $E_0(k)$ is the energy of the exciton in the absence of lattice fluctuations. \hat{H}_p denotes the phonon energies and $b_q^\dagger (b_q)$ is the creation (annihilation) phonon operator with frequency $\omega(q)$ and wavevector q . The exciton-phonon interaction operator, \mathcal{H}_{ep} involves the respective electron-phonon and hole-phonon coupling functions, χ_e and χ_h .

The initial state consisting of an exciton and a composite condensate of bi-fermion pairs with zero center-of-mass momentum appear as^{31,42-44}

$$|\Phi_i\rangle = C_K^\dagger \prod_k \left[u(k) + v(k) a_k^\dagger h_{-k}^\dagger \right] |0\rangle \quad (31)$$

where the exciton possesses a center-of-mass momentum K and an internal motion described by the wave function ϕ_{1s} which appears in Eq. 21. The final scattered state becomes

$$|\Phi_f\rangle = \prod_k \left[u'(k) + v'(k) a_k^\dagger h_{-k}^\dagger \right] |0\rangle, \quad (32)$$

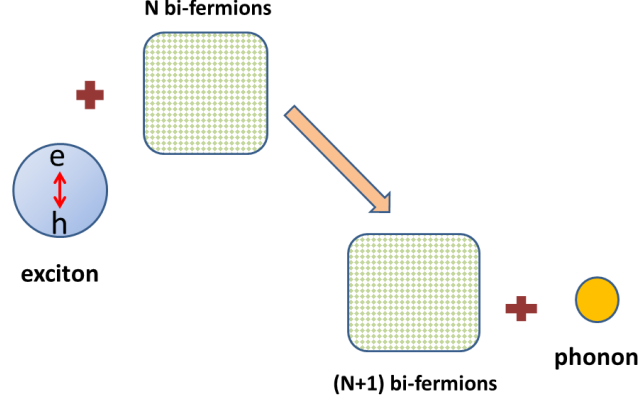


FIG. 1: Schematics of a channel in which an initial state consisting of an exciton and a composite condensate of N bi-fermion pairs is scattered to a final state of $N + 1$ bi-fermions pairs, with emission of a phonon.

where $\sum_k |v'(k)|^2 \approx 1 + N$, so that $N + 1$ bi-fermion pairs are present in the final state. In the limit of very large N and low density condensates, $\frac{u(k)}{u(k')} \approx 1$ and $\frac{v(k)}{v(k')} \approx 1$, irrespective of the value of k .

The rate of scattering (R_s) of the process shown in Fig.1 can be obtained using the Fermi Golden Rule^{22,23,25,31}, assuming a large exciton momentum K . This ensures that there is no backflow of information from the reservoir due to short memory bath times, which allows the use of the Born-Markov approximation

$$R_s = \frac{2\pi N}{\hbar} \sum_q |\chi_e(2q)\phi_{1s}(q) + \chi_e(2q)\phi_{1s}(-q)|^2 \alpha_{N+1}^2 \delta(\hbar\omega_i - \hbar\omega_f - \hbar\omega_o) \quad (33)$$

where α_{N+1}^2 (using Eq. 26) quantifies the effective probability of increasing the number of bi-fermion pairs from a size of N to $N + 1$. $\hbar\omega_i$ ($\hbar\omega_f$) denotes the energy of the initial (final) energy of the scattered system, and $\hbar\omega_o$ is the energy of the emitted phonon. In general, Eq. 33 is applicable to small bosonic deviations which appear at low bosonic densities, with simplification also introduced by neglecting the k -dependence of the excitonic wave function from coherence terms such as $|u^*(k)v(k)|^2$. The upper bound for α_{N+1}^2 (see Eq. 7), indicates that the rate of scattering R_s decreases with increase in purity P , in agreement with decreased probabilities of charge carriers relaxing to unoccupied states due to the Pauli exclusion principle.

Based on the decrease of $\frac{\chi_{N+1}}{\chi_N}$ with N , we can conclude that the rate R_s decreases with increase in N for bi-fermion cobosons. The absence of phase-space of charge carriers, particularly near the Fermi level, results in an inhibition of stimulated scattering processes when coherence between the bi-fermion pair states is decreased. There is the possibility that an uncorrelated electron-hole pair may bind to form an exciton, with emission of phonons, however this process is less likely to occur in bi-fermion condensates of high P values. As observed in an earlier work³¹, the spontaneous and stimulated scattering rates decrease at larger densities at which greater deviations from ideal bosonic behavior occur (at increased values of P). In the limit of an electron-hole plasma state, $\alpha_{N+1}^2 \rightarrow 0$, and an absence of stimulated emission is predicted.

The appearance of the normalization ratio, α_{N+1}^2 in Eq. 33 is the main result of this work. This ratio captures the role of the Pauli exclusion principle at the point when there is competition for single-fermion states. In an initial state, the N bi-fermions could occupy the modes $j_1 \dots j_N$, and the incoming $N + 1$ st coboson may need to be accommodated among the remaining $S - N$ unoccupied Schmidt modes. The effective probability that the incoming bi-fermion occupies an initially unoccupied Schmidt mode is evaluated by adding all coefficients associated with the unoccupied mode configurations which is given by $\sum_{m \in j_{N+1}, \dots, j_S} \lambda_m$. This process has to be repeated for each configuration of j_1, \dots, j_N to yield the final probability to add an $N + 1$ st coboson to an N -coboson which is given by the normalization ratio, α_{N+1}^2 . A redistribution among the bi-fermion Schmidt modes may occur as a result of scattering processes, including those with no phonon emission, and the normalization ratio may be affected by the outgoing phonon energies. Such possibilities need greater examination in future works.

Accurate values of α_{N+1}^2 are generally not easily computable for two-fermion wavefunctions and large number N of bi-fermion pair systems, however the bounds obtained in Ref.²⁰ do resolve the computational demands associated with large boson systems. An alternative measure that can be used to assess the scattering process involves incorporation of the fluctuations in the mean number, $\langle \hat{N} \rangle$ (Eq.17) in the rate expression, R_s (Eq.33). The scattering process is optimized when fluctuations in the exciton number vanish in the limit $P \rightarrow 0$, due to the availability of a maximum number of ideal bosonic excitons for

interaction with the phonons. The qualitative predictions here may be tested following the experimental work of Mondal et. al.⁴⁷ who investigated the dynamics of state-filling dynamics in self-assembled InAs/GaAs quantum dots (QDs) using picosecond excitation-correlation (EC) spectroscopy. The action of the Pauli exclusion principle appeared visible in the photoluminescence results⁴⁷. Future experimental works may wish to examine the controlled scattering of excitons which occupy specific Schmidt modes, and the subsequent emission of phonons with a desired range of energies.

The strong relationship between quantum entanglement of the constituents of boson systems and their bosonic quality therefore play an important role in the scattering process depicted in Fig. 1, and as seen in the rate R_s of Eq. 33. The usefulness of the normalization term may be studied in scattering processes involving other generalized composite models, such as bi-bosons which are made up of smaller boson fragments¹⁹. The scattering dynamics which occurs in the case of bi-boson systems will be considered in Sec. V

C. Application to the dynamics of singlet and triplet excitons

In strategic polymer materials, the dynamics of exciton is determined by the kinetic transformation involving singlet and triplet excitonic states^{48,49}. While singlet excitons are emissive and account for electroluminescence in conjugated polymers, triplet excitons remain non-emissive and these differences in optical properties give rise to a range of electroluminescence efficiencies in polymers. It is therefore worthwhile to provide brief mention of the extension of the scattering rate in Eq.33 to excitons which can form in the singlet or triplet state, depending on the spin angular momentum. It is known that four spin eigenstates can result from the electron-hole quasi-particle based on the spin angular momentum operator S , and its z -component, S_z as follows as

$$\begin{aligned} (1) \quad & a_{\uparrow} h_{\uparrow} \\ (2) \quad & \frac{1}{\sqrt{2}}(a_{\downarrow} h_{\uparrow} + h_{\downarrow} a_{\uparrow}) \\ (3) \quad & a_{\downarrow} h_{\downarrow} \\ (4) \quad & \frac{1}{\sqrt{2}}(a_{\downarrow} h_{\uparrow} - h_{\downarrow} a_{\uparrow}) \end{aligned} \tag{34}$$

The first three symmetric eigenstates of the triplet exciton in Eq. 34 are associated with $S=1$, while the last anti-symmetric state of the singlet exciton is linked to $S=0$. Due to the Pauli exclusion principle, the triplet state is correlated with the anti-symmetric spatial wavefunction, while the singlet state is linked with the symmetric spatial wavefunction. On this basis, differences in the probabilities of occupation of Schmidt modes of singlet and triplet excitons are to be expected, with likely variations in the scattering rates for the two types of excitons. Important mechanisms such as the scattering of the triplet exciton into the singlet exciton state via acoustic phonons, as well as the fission of a singlet exciton into two triplet excitons⁵⁰ are similarly expected to be influenced by the dependence of χ_{N+1}/χ_N on S . A detailed examination of the exact dependence of the normalization ratio χ_{N+1}/χ_N , which governs the scattering rate in Eq. 33, on the operator S will be considered in future works.

V. COMPOSITE BOSON MADE OF TWO BOUND BOSONIC CONSTITUENTS (BI-BOSONS)

The multiple occupation of single constituents in a specific mode for bi-bosons is not compromised due to Pauli-blocking as is evident in Eq. 4. The bi-boson operator, $d_j^\dagger := a_j^\dagger b_j^\dagger$, satisfies¹⁹

$$[d_j^\dagger, d_k^\dagger] = \delta_{j,k}(1 + 2n_j) \tag{35}$$

as well as the over-normalization relation, $[d_j^\dagger]^N |0\rangle = N! |N\rangle_j$ ¹⁹. where n_j denotes the number of bi-bosons in the j th mode. These relations highlight the enhanced bunching tendencies of the two-boson composites as there can be multiple occupation of a single Schmidt mode. The normalization ratio for bi-boson composites appear as¹⁹

$$PN + 1 \leq \frac{\chi_{N+1}}{\chi_N} \leq \sqrt{PN + 1}, \tag{36}$$

which may be compared to Eq. 7 for bi-fermion type bosons. The relation in Eq. 36 is not saturable, however a relation with tight bounds is not in the simple form provided here.

In bi-boson cobosons, there are two regimes associated with $N\sqrt{P} \ll 1$ and $N\lambda_1 \gg 1$ ¹⁹ where λ_1 is the largest Schmidt coefficient. In the latter regime, the Schmidt modes with magnitude λ_1 are favorably populated resulting in the characteristic super-bunching tendency of bi-bosons. As the number of composites N is increased, a Schmidt mode that is occupied by a boson is likely to attract further occupation due to the n_j dependency in Eq. 35. The increase in the effective boson number in

the favored macroscopically occupied Schmidt modes occurs at the expense of bosons distributed in other modes or present in adjacent ortho-complement subspaces.

The bunching attributes of bi-bosons has implications for scattering processes as an incoming boson species that collides with the main coboson target is likely to occupy the macroscopically occupied Schmidt mode resulting in an increased rate. In this regard, the scattering may differ from that involving a composite boson system of bi-fermion pairs where the scattering rate decreases with increase in N bi-fermions. For scattering of phonons of select energies, there may be enhanced scattering of bi-bosons at conditions favorable to super-bunching (such as large N) which can be deduced using Eqs.33 and 36.

The quantum droplet formed from electron-hole aggregates³² promises as a suitable platform to test the quantum mechanical features such as bunching attributes of bi-bosons, under given experimental conditions. For instance, two excitonic droplets may be deposited in spatially separated quantum wells, and depending on the inter-well tunneling strengths and intra-well bosonic interactions, the presence of superbosonic features under controlled conditions may be probed. Likewise the enhanced scattering properties of bi-bosons involving phonons in integrated circuits that are subject to lattice vibrations, could also be investigated in future experimental works.

VI. CONCLUSION AND OUTLOOK

In this paper, we have examined the influence of Pauli-exclusion of fermions when composite bosons of bi-fermion pairs undergo scattering due to interactions with phonons. The entanglement between the fermionic constituents explicitly enters in the scattering rate of the composites. Large entanglement ($P \ll 1/N$) is synonymous for ideal bosonic behavior, while smaller entanglement leads to phase-space-filling effects, with reduced scattering. Composite bosons characterized by larger purities (with high densities of bosons), have decreased scattering due to the phase-space filling effect, where there is decreased probabilities of charge carriers relaxing to unoccupied states. The demonstration of the dependence of the scattering rate on the normalization ratio, α_{N+1}^2 highlights the usefulness of the derived scattering rate in the investigation of generalized bosonic systems with multiple condensates such as quantum droplets³².

When the composite boson under consideration is made of smaller boson fragments such as in the case of bi-bosons, the scattering process is predicted to reveal features that are qualitatively different from those involving bi-fermion cobosons. In particular, due to super-bunching properties of bosons occupying macroscopically occupied Schmidt modes, there may be enhanced scattering linked to specific modes. The results of this work contributes to fundamental aspects of quantum mechanical modeling of composite boson systems. This study has potential application in Bose-Einstein condensates in confined systems, and in the control of inter-bosonic carrier-carrier interactions in photovoltaic technologies that rely on the mechanism of multiple exciton generation (MEG)^{51,52}. The Pauli exclusion principle is also expected to dominate exciton dynamics in layered transition metal dichalcogenides with show rich excitonic features^{53–55}. To this end, the exclusion principle may be examined in layered semiconductor systems in future works.

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